Karlsruhe Institute of Technology

Chemistry of Oxydic and Organic Interfaces
Institute of Functional Interfaces

A novel series of surface attached metal-organic frameworks by liquid phase epitaxy

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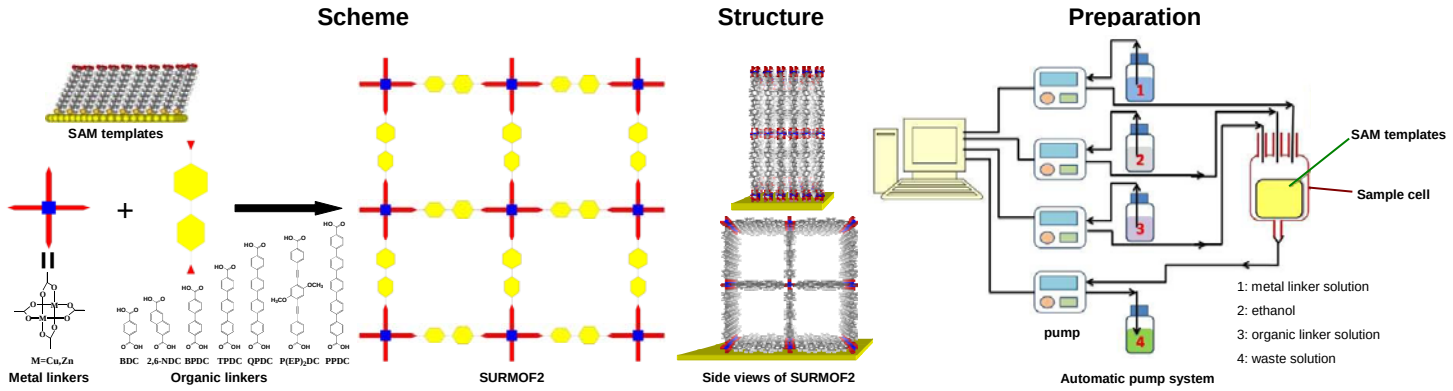
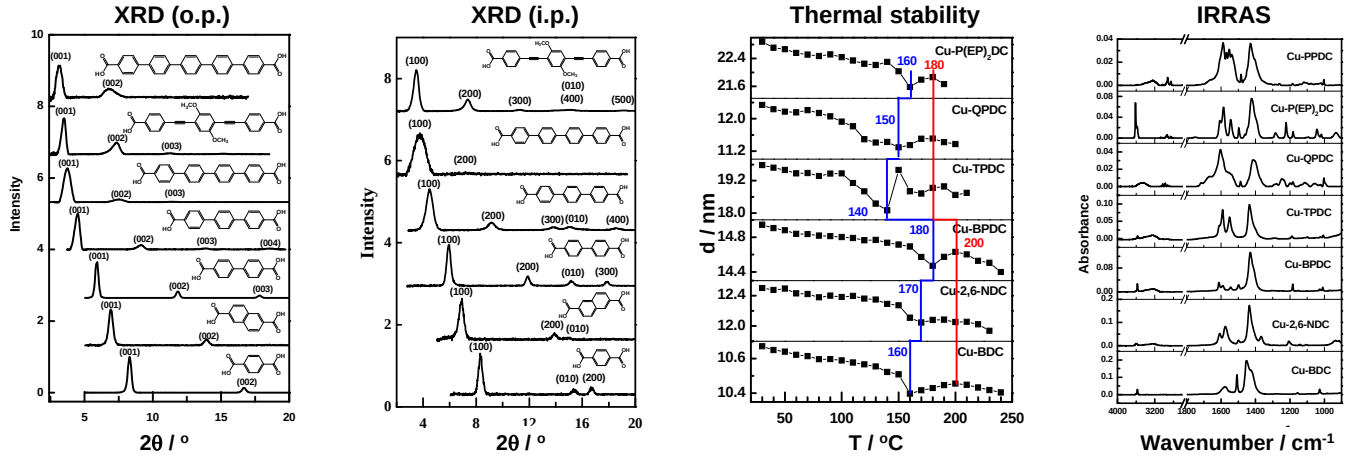
Introduction

MOF thin films [1–2] are of special importance in particular with regard to electrochemistry, sensor technology, in electronic devices as well as biocompatible substrates. The liquid-phase epitaxy is an important to fabricate highly orientated MOF coatings with well-defined thickness and the absence of pin-hole defects.

Liquid Phase Epitaxy

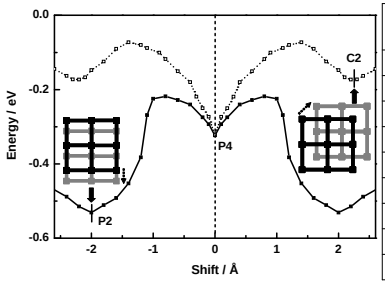


Experimental



The XRD data show that well-orientated 2D-MOF thin films are grown on COOH-terminated SAM surface along (001) direction with high thermal stability up to 200 ° C. The OH stretchings observed in IRRAS spectra demonstrate that these 2D-MOF thin films contain water molecules coordinated to the axial position of paddle-wheel Cu.

Calculation



	Symmetry	a= c	b	Stacking Energy (eV)
$Cu_2(BDC)_2$	C2	11.19	5.0	-0.76
$Cu_2(BDC)_2$	P2	11.19	5.4	-0.8
$Cu_2(BDC)_2$	P4	11.19	5.8	-0.59
$Cu_2(BDC)_2$	P2	13.35	5.6	-0.4
$Cu_2(BPDC)_2$	P4	15.49	5.9	-0.68
$Cu_2(TPDC)_2$	P4	19.84	5.9	-0.91
$Cu_2(QPDC)_2$	P4	24.24	5.9	-1.21
$Cu_2(P(EP)_2DC)_2$	P4	25.12	5.2	-1.73
$Cu_2(PPDC)_2$	P4	28.59	5.9	-1.45

Conclusion

A novel series of high thermal stable and variable pore sizes of SURMOF2 thin films are successfully fabricated by LPE. The calculation shows that these thin films are metastable structures with P4 symmetry, which can be accessed by LPE method.

1. Shekhah, O.; Liu, J.; Fischer, R.A.; Wöll, C. MOF thin films: Existing and future applications. *Chem. Soc. Rev.* **2011**, *40*, 1081–1106.
2. Zacher, D.; Shekhah, O.; Wöll, C.; Fischer, R.A. Thin films of metal-organic frameworks. *Chem. Soc. Rev.* **2009**, *38*, 1418–1429.